# Optimization of a Thin Film Solar Cell with Metallic Nanoparticles

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*Abstract*— In this paper the authors optimize the geometry of a thin solar cell with metallic nanoparticles by employing a finite element code to compute the light scattering from the cell and genetic algorithm optimization.

*Index Terms*— Photovoltaic cells, Nanoparticles, Genetic Algorithms, Scattering, Computational electromagnetics, Finite element methods.

## I. INTRODUCTION

The study of the efficiency of solar cells made of photovoltaic (PV) layers is very important to the aim of reduce the use of fossil fuels.

Recently several researchers have demonstrated that the insertion of metallic nanoparticles within or near PV layers may improve significantly the efficiency of the solar cells.

In this paper the authors optimize the geometry of a thin solar cell by employing an FEM code to compute the light scattering from the cell and suitable genetic algorithms (GAs) for optimization.

### II. FEM ANALYSIS OF LIGHT SCATTERING

Consider the thin film solar cell depicted in Fig. 1, in which hemi-ellipsoidal metallic nanoparticles, having semi-axes a, b and c, with a=b>c, are placed near a PV layer, having a thickness t. The particles centers are regularly placed at the nodes of a rectangular grid exhibiting the same grid step 2d along the x- and y-axis. To simplify the optimization the particles are assumed to have a given volume V=2abc/3, so that only one degree of freedom specifies their shape.

A monochromatic electromagnetic plane wave at optical frequency is incident normally on this system. For the sake of simplicity we assume that the wave is E-polarized along the x-axis.

For this electromagnetic scattering problem the Helmholtz vector equation holds:

$$\nabla \times \left(\mu_{\rm r}^{-1} \nabla \times \overline{\rm E}\right) - k_0^2 \varepsilon_{\rm r} \overline{\rm E} = 0 \tag{1}$$

where  $\mu_r$  and  $\epsilon_r$  are the relative magnetic permeability and electrical permittivity, respectively and  $k_0$  is the free-space wavenumber, given by:

$$\mathbf{k}_0 = \omega \sqrt{\varepsilon_0 \mu_0} , \qquad (2)$$

with  $\omega$  being the angular frequency and  $\mu_0$  and  $\epsilon_0$  the free-space permeability and permittivity, respectively.

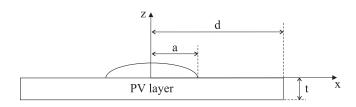


Fig. 1. Solar cell with a hemi-ellisoidal metallic nanopartcle.

For symmetry reasons the analysis can be restricted to the domain 0 < x < d, 0 < y < d, by imposing homogeneous Dirichlet boundary conditions on the x=0 and x=d planes and homogeneous Neumann ones on the y=0 and y=d planes. On the z direction the domain is truncated by means of two PML layers (not shown in Fig.1), one over and one under the cell. The analysis domain is discretized by means of tetrahedral edge finite elements.

At optical frequencies the metallic nanoparticles give rise to plasmons oscillations, which are taken into account by modeling the metal by means of a complex relative electric permittivity (Drude model) [1], given by:

$$\varepsilon_{\rm r} = -\frac{\omega_{\rm p}^2 - (\omega^2 + \nu^2)}{\omega^2 + \nu^2} - j \frac{\nu \omega_{\rm p}^2}{\omega(\omega^2 + \nu^2)}$$
(3)

where  $\omega_p$  is the plasma frequency of the free electrons and v is the relaxation frequency, the values of which are experimentally determined [2]. Note that at the optical frequencies of interest, the real part of the relative electric permittivity is negative. Assuming a unitary relative magnetic permeability, the FEM analysis is easily performed [3, 4].

In postprocessing the following non dimensional quantity is computed:

$$f(a,d,t) = \frac{W_{i} - W_{o} - W_{j}}{S_{inc}d^{2}}$$
(4)

where  $W_i$  is the flux of the Poynting vector through a square surface over the cell,  $W_o$  is the same flux through a square surface under the cell,  $W_j$  is the Joule loss in the metallic particle and  $S_{inc}$  is the Poynting vector module of the incident wave.

#### III. OPTIMIZATION BY GENETIC ALGORITHMS

By employing the quantity in (4) as objective function to be maximized, a stochastic optimization is started by assuming the following data:

Metal of the nanoparticles: silver	
Nanoparticle volume	$V = 25600 \text{ nm}^3$
Light Wavelengtht:	$\lambda = 900 \text{ nm}$
PV layer permittivity:	$\epsilon_r=4$
PV layer permeability:	$\mu_r = 1$

The geometrical parameters to be optimized are assumed to vary in the following ranges:

$$25 \text{ nm} < a < 55 \text{ nm}$$
  
 $40 \text{ nm} < d < 250 \text{ nm}$   
 $5 \text{ nm} < t < 100 \text{ nm}$ 

The stochastic optimization was pursued by means of Genetic Algorithms (GAs), which are search algorithms which simulate the random evolution of populations of biological entities. These well-known algorithms have proven to be very efficient in optimizing electromagnetic devices [5, 6] both for low and high frequency applications. In this paper GAs have been used with the following characteristics [7]:

Population size: P=30 Number of generations: Ng=30 Binary lengths: Na=5, Nd=7, Nt=6 Selection: tournament selection with elitism Crossover type: two-point crossover Crossover probability at generation k:  $Pc_k = 0.3 + 0.4(k-1)/(Ng-1)$ Mutation probability at generation k:  $Pm_k = 0.05 - 0.04(k-1)/(Ng-1)$ 

As far as representation is concerned, the three geometric variables a, d, and t, were coded into binary strings of five, seven and six bits, respectively, giving a total of N=18 bits.

The reproduction process, which randomly creates a new generation from the old one, was chosen by tournament selection with a shuffling technique to choose random pairs.

The crossover process, by means of which individuals exchange chromosomes from one generation to the other, was two-point crossover with a probability  $P_c$  linearly varying from 0.3 to 0.7 while optimization goes on.

The mutation process, by means of which some random flips in the chromosomes of an individual are made, was employed with a probability  $P_m$  linearly decreasing from 0.05 to 0.01 while optimization proceeds.

The evolution was halted after 30 generations, reaching an optimal function value  $f_{max}$ =3.011, in relation to the following parameter configuration (values rounded to 0.5 nm):

 $a = 42 \text{ nm}, \quad d = 61.5 \text{ nm}, \quad t = 11 \text{ nm}$ 

In Fig. 2 the best (maximum) values of the objective function are plotted through the various generations. Fig. 3 shows the behaviour of (4) vs. wavelength (nm) for the best configuration.

The computations were performed by means of ELFIN, a large FEM code developed by the authors for electromagnetic CAD research [8].

More details and example will be provided in the full paper.

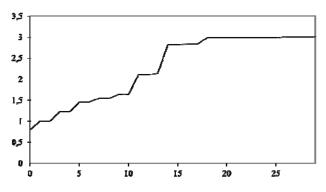


Fig. 2. Best objective function f over GA generations.

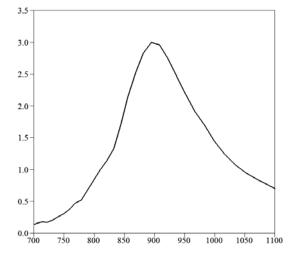


Fig. 3. Values of f vs. wavelength (nm) for the best configuration.

#### ACKNOWLEDGEMENTS

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#### REFERENCES

- C. F. Bohren and D. R. Huffman, Absorption and Scattering of Light by Small Particles, Wiley, 1983
- [2] P.B. Johnson and R. W. Cristy, "Optical constants of the noble metals", *Phys. Rev. B*, vol 6, pp. 4370-4379, 1972.
- [3] S. Alfonzetti, G. Borzì, "Finite element solution to electromagnetic scattering problems by means of the Robin boundary condition iteration method," *IEEE Transactions on Antennas and Propagations*, vol. 50, n. 2, pp. 132-140. February 2002.
- [4] G. Aiello, S. Alfonzetti, V. Brancaforte, V. Chiarello, N. Salerno, "Applying FEM-RBCI to the analysis of plasmons in metallic nanoparticles", *International Journal of Applied Electromagnetics and Mechanics (IJAEM)*, vol. 39, n. 1-4, pp. 13-20, 2012.
- [5] S. Russenschuck, "Synthesis, inverse problems and optimization in computational electromagnetics," *Int. J. Numer. Modelling: Electronic Networks, Devices and Fields*, vol. 9, pp. 45-57, January-April 1996.
- [6] P. G. Alotto, et alii, "Stochastic algorithms in electromagnetic optimization," *IEEE Transactions on Magnetics*, vol. 34, pp. 3674-3684, Sept. 1998.
- [7] S. Alfonzetti, E. Dilettoso, N. Salerno, "A proposal for a universal parameter configuration for genetic algorithm optimization of electromagnetic devices," *IEEE Transactions on Magnetics*, vol. 37, n. 5, pp.3208-3211, September 2001.
- [8] G. Aiello, S. Alfonzetti, G. Borzì, and N. Salerno, "An overview of the ELFIN code for finite element research in electrical engineering", in *Software for Electrical Engineering Analysis and Design*, A Konrad & C. A. Brebbia (ed.), WIT Press, Southampton (U.K.), 1999.